

**Table B-3: Arnot & Gobas Equations**

Biological			
Component	Symbol	Units	Equation
Chemical concentration in the organism	$C_B$	pg/kg <del>ww</del> ww	$C_B = \{k_1 * (m_O * C_{WD} + m_P * C_{WD,P}) + k_D * \sum P_i * C_{D,i}\} / (k_2 + k_E + k_C + k_M)$ <b>Equation 1</b>
Chemical concentration in prey item <i>i</i>	$C_{D,i}$	pg/kg ww	same as above; included to indicate that the general equation is also used to estimate chemical concentrations in prey species <b>Equation 1</b>
Organism-water partition coefficient on a wet weight basis	$K_{BW}$	unitless	$K_{BW} = k_1 / k_2 = V_{LB} * K_{OW} + V_{NP} * \beta * K_{OW} + V_{WP}$ <b>Equation 2</b>
Rate constant for aqueous uptake (fish, invertebrates and zooplankton)	$k_1$	L/kg/day	$k_1 = E_w * G_v / W_B$ <b>Equation 4</b>
Gill ventilation rate	$G_v$	L/d	$G_v = 1400 * W_B^{0.65} / C_{Ox}$ <b>Equation 5</b>
Respiratory surface chemical uptake efficiency	$E_w$	unitless	$E_w = (1.85 + (155 / K_{ow}))^{-1}$ <b>Equation 7</b>
Rate constant for aqueous uptake (algae, phytoplankton and aquatic macrophytes)	$k_1$	L/kg/day	$k_1 = (A + (B / K_{ow}))^{-1}$ <u>(A and B values from literature)</u> <b>Equation 8</b>
Rate constant for chemical elimination via the respiratory area (gill)	$k_2$	day <sup>-1</sup>	$k_2 = k_1 / K_{BW}$ <b>Equation 9</b>
Phytoplankton-water partition coefficient on a wet weight basis	$K_{PW}$	unitless	$K_{PW} = V_{LP} * K_{OW} + V_{NP} * 0.35 * K_{OW} + V_{WP}$ <b>Equation 10</b>
Rate constant for chemical uptake via ingestion and digestion of food and water	$k_D$	kg food/kg organism/day	$k_D = E_D * G_D / W_B$ <b>Equation 11</b>
Dietary chemical transfer efficiency	$E_D$	unitless	$E_D = (3.0 * 10^{-7} * K_{OW} + 2.0)^{-1}$ <b>Equation 12</b>
Feeding rate - other species	$G_D$	kg/d	$G_D = 0.022 * W_B^{0.85} * e^{(0.006 * T)}$ <b>Equation 13</b>
Feeding rate - filter-feeders	$G_D$	kg/d	$G_D = G_v * C_s * \sigma$ <b>Equation 14</b>

**Commented [BLJ1]:** Changed case to be consistent with rest of document.

**Commented [BLJ2]:** Two Equation 1's

**Commented [BLJ3]:** No Equation 3 (OK. I found it below. Perhaps you should put an empty row here and indicate in that row that "(Equation 3 is found below in the discussion of chemical model components)" Alternatively, perhaps it would better to renumber equations.

**Commented [BLJ4]:** No Equation 6. (See comment on equation 3 above.)

**Commented [BLJ5]:** No decimal point in original. Is this correct?

**Commented [BLJ6]:** Sigma term not defined. Might there be other terms in this table that are similarly not defined??

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Component	Symbol	Units	Equation
Rate constant for chemical elimination via excretion into egested feces	$k_E$	day <sup>-1</sup>	$k_E = G_F \cdot E_D \cdot K_{GB} / W_B$ <b>Equation 15</b>
Partition coefficient of the chemical between the contents of the gastrointestinal tract and the organism	$K_{GB}$	unitless	$K_{GB} = (V_{LG} \cdot K_{OW} + V_{NG} \cdot \beta \cdot K_{OW} + V_{WG}) / (V_{LB} \cdot K_{OW} + V_{NB} \cdot \beta \cdot K_{OW} + V_{WB})$ <b>Equation 16</b>
Fecal egestion rate	$G_F$	kg/d	$G_F = \{ (1 - \delta_L) \cdot V_{LD} + (1 - \varepsilon_L) \cdot V_{ND} + (1 - \varepsilon_N) \cdot V_{WD} \} \cdot G_D$ <b>Equation 17</b>
Lipid fraction of gut contents	$V_{LG}$	kg lipid/kg digesta ww	$V_{LG} = (1 - \varepsilon_L) \cdot V_{LD} / [(1 - \varepsilon_L) \cdot V_{LD} + (1 - \varepsilon_N) \cdot V_{ND} + (1 - \varepsilon_W) \cdot V_{WD}]$ <b>Equation 18</b>
NLOM fraction of gut contents	$V_{NG}$	kg NLOM/kg digesta ww	$V_{NG} = (1 - \varepsilon_L) \cdot V_{ND} / [(1 - \varepsilon_L) \cdot V_{LD} + (1 - \varepsilon_N) \cdot V_{ND} + (1 - \varepsilon_W) \cdot V_{WD}]$ <b>Equation 19</b>
Water fraction of gut contents	$V_{WG}$	kg water/kg digesta ww	$V_{WG} = (1 - \varepsilon_L) \cdot V_{WD} / [(1 - \varepsilon_L) \cdot V_{LD} + (1 - \varepsilon_N) \cdot V_{ND} + (1 - \varepsilon_W) \cdot V_{WD}]$ <b>Equation 20</b>
Rate constant for growth of aquatic organisms	$k_G$	day <sup>-1</sup>	$k_G = 0.0005 \times W_B^{-0.2}$ <b>Equation 21</b>
Rate constant for metabolic transformation of chemical	$k_M$	day <sup>-1</sup>	Metabolism of PCB and DDE are not expected to be significant for application of the model to Portland Harbor. Estimates for $k_M$ were, however, identified in the model calibration process
Overall lipid content of the diet	$V_{LD}$	kg lipid/kg food ww	$V_{LD} = \sum P_i \cdot V_{LB,i}$ <b>Total dietary lipid</b>
Overall NLOM content of the diet	$V_{ND}$	kg NLOM/kg food ww	$V_{ND} = \sum P_i \cdot V_{NB,i}$ <b>Total dietary non-lipid organic matter</b>
Overall water content of the diet	$V_{WD}$	kg water/kg food ww	$V_{WD} = \sum P_i \cdot V_{WB,i}$ <b>Total dietary water</b>
<b>Chemical</b>			
Component	Symbol	Units	Equation
Bioavailable Solute Fraction	$\phi$	unitless	$\phi = 1 / (1 + \chi_{POC} \cdot D_{POC} \cdot \alpha_{POC} \cdot K_{OW} + \chi_{DOC} \cdot D_{DOC} \cdot \alpha_{DOC} \cdot K_{OW})$ <b>Equation 3</b>
Dissolved oxygen concentration of water (RM 2 to RM 11)	$C_{OX}$	mg O <sub>2</sub> /L	$C_{OX} = (-0.24 \cdot T + 14.04) \cdot 0.9$ <b>Equation 6</b>

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Component	Symbol	Units	Equation
Freely dissolved chemical concentration in the pore water	$C_{WD,P}$	ng/L	$C_{WD,P} = C_{S,OC} * f_{OCs} / K_{OC}$  <b>Equation 22</b>
Chemical concentration in the sediment, organic carbon normalized	$C_{S,OC}$	pg/kg dw OC	$C_{S,OC} = C_S / OC_{Sed}$  <b>Equation 23</b>
Freely dissolved chemical concentration in the water (total PCBs as congeners and 4,4'-DDE)	$C_{WD}$	ng/L	$C_{WD} = C_{WT} * \phi$  (See Equation 1)
Organic carbon-water partition coefficient (total PCBs as Aroclors and 4,4'-DDE)	Log $K_{OC}$	unitless	$\text{Log } K_{OC} = \text{Log}_{10}(0.35 * 10^{\text{Log } K_{OW}})$

**Commented [BLJ7]:** I don't believe this is defined elsewhere. (I found it in text, but perhaps it could be defined here as well to make table useful independent of text.)